

## Self-Replicating Silane Films: Structure and Water Intercalation

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Abstract No. ocko6929

Beamline(s): X22A

**Introduction:** Molecular self-assembly at liquid-solid interfaces is gaining increasing importance as an advanced approach to the construction of solid-supported mono- and multi-layer structures with well defined organization of their molecular components. Recently, a self-replicating, geometric growth process was discovered for silanes in which the film thickness doubles during every chemical cycle[1]. Using this method, films up to 32 layers thick have been successfully grown. A better understanding of the internal structure of these films should help explain the novel growth process.

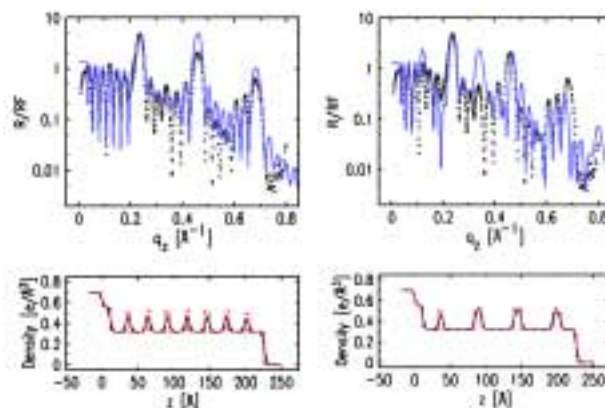
**Methods and Materials:** Self-replicating, 8 layer thick octadecyltrichlorosilane (OTS) were prepared using the method described by Maoz[1]. This multi-step process involves the intercalation of water and the replacement of water by “silane bilayers”. X-ray reflectivity and GID studies have been carried out on these films under dry and wet environments.

**Results:** Our results demonstrate that these multi-layer silane films are of high quality with Å scale roughness. Under dry conditions, the overall film thickness, determined from the spacing of the Kiessig fringes, is in agreement with an 8 layer thick film of extended molecules. However, the internal structure cannot be described by uniform bilayers, as expected [1]. The bilayer structure would give rise to strong half-order diffraction features and these are not observed in the reflectivity profiles (see figure 1). The data is better described by a monolayer density profile (left) rather than by simple bilayers (right). However, on the basis of the existing data it is difficult to distinguish between a simple monolayer model and an effective monolayer model where the local structure is composed of bilayers with a spatially modulated bilayer phase. In either case, the average thickness of each layer is 27.5 Å, consistent with the expected OTS molecular length.

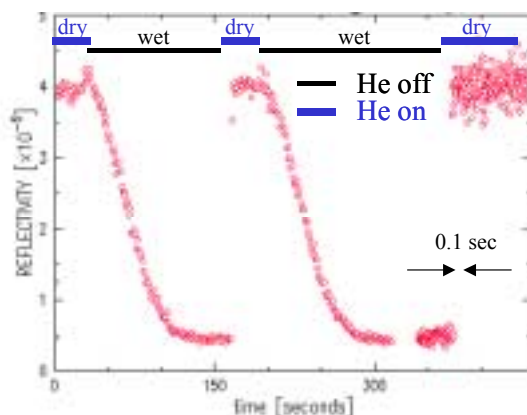
In order to understand the role of water in the self-replicating growth process, we have carried out reflectivity measurements under both dry and saturated humidity conditions. The reflectivity curves under both conditions are similar, albeit the layers expand by 1.5 Å under humid conditions, corresponding to one molecule of water per molecule of OTS. We have also carried out kinetic studies of the water intercalation process by measuring the reflectivity at a fixed position versus time while the humidity in the cell is suddenly changed. Our results (see figure 2) show that the water diffusion into the layers occurs in less than 0.1 seconds.

**Acknowledgments:** This work is supported by US-Israeli Binational Science Foundation and the U.S. Department of Energy, Office of Basic Energy Science.

**References:** [1] R. Maoz, S. Matlis, E. DiMasi, B.M. Ocko, and J. Sagiv, *Nature* **384**, 150 (1996).



**Figure 1.** Normalized reflectivity from an 8 layer, self-replicating silane film, along with the calculated reflectivity curves (blue lines) from the density models given below. The monolayer model is shown on the left and the bilayer model is shown on the right.



**Figure 2.** Kinetics of water intercalation after a sudden change in the humidity at a fixed position on the reflectivity curve